A NOVEL ALGORITHM FOR SOLVING THE TRUE COINCIDENT COUNTING ISSUES IN MONTE CARLO SIMULATIONS FOR RADIATION SPECTROSCOPY

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Abstract—**Coincident counts can be observed in experimental radiation spectroscopy. Accurate quantification of the radiation source requires the detection efficiency of the spectrometer, which is often experimentally determined. However, Monte Carlo analysis can be used to supplement experimental approaches to determine the detection efficiency a priori. The traditional Monte Carlo method overestimates the detection efficiency as a result of omitting coincident counts caused mainly by multiple cascade source particles. In this study, a novel "multi-primary coincident counting" algorithm was developed using the Geant4 Monte Carlo simulation toolkit. A high-purity Germanium detector for ^{60}Co gamma-ray spectroscopy problems was accurately modeled to validate the developed algorithm. The simulated pulse height spectrum agreed well qualitatively with the measured spectrum obtained using the high-purity Germanium detector. The developed algorithm can be extended to other applications, with a particular emphasis on challenging radiation fields, such as counting multiple types of coincident radiations released from nuclear fission or used nuclear fuel.**

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Key words: ^{60}Co; detector, germanium; Monte Carlo; Spectroscopy, gamma

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INTRODUCTION

DUE TO its high-energy resolution characteristics, the high-purity Germanium (HPGe) detector is the most widely used gamma-ray spectroscopy system for isotopic analysis. Once the radionuclide is identified according to the peak energy in the calibrated pulse height spectrum, the absolute intensity or activity of the source can be determined from the counting time, the counts under the full-energy peak, and the absolute detection efficiency of the detector for this specific gamma-ray energy. Hence, prior knowledge of the detector response to different gamma-ray energies is required before quantifying an unknown gamma-ray source.

The efficiency response curve (absolute detection efficiency vs. photon energy) of the detector can be determined experimentally if enough gamma sources covering a large range of photon energies are available for measurement. For cases in which specific sources are not available, theoretical calculation is an effective alternative to determine the detector response.

Monte Carlo (MC) simulation is the most commonly used method of calculating the theoretical responses of the detector for different photon energies. Nevertheless, because of the existence of the intrinsic discrepancies in particle source specification and counting principles between the traditional Monte Carlo simulation and the experimental measurement, discrepancies always exist between the simulated and measured spectra. The degree of discrepancy depends on the physics models and counting algorithms applied in the simulation and the pulse signal output mechanism in the detector.

The biggest discrepancy comes from the "summation effect" caused by the coincident detection of two or more gamma rays. This effect can result in the appearance of the extended counting continuum beyond the maximum full-peak energy and sum peak(s) in the measured spectrum. There are two common types of coincidences. One is the "true coincidence," caused by the multiple cascade gamma rays emitted from the same radionuclide per disintegration. The other is the "chance coincidence," caused by the accidental combination of two or more separate gamma rays from independent disintegrations occurring closely spaced in time. If a second pulse arrives within the resolving time of the detector following a typical signal pulse, the

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detector cannot separate these two pulses and produces only one signal with the intensity (height) equal to the sum of these two pulses (Knoll 2010).

In detecting a single radioactive source emitting multiple cascade gamma rays, the true coincident counting effect is observed in the measured pulse height spectrum and thus decreases the detection efficiency for each specific gamma ray. Due to its inability to process the coincident counts, the traditional MC method always overestimates the detection efficiency. This overestimation has been reported by some researchers (Vasconcelos et al. 2011). A coincidence correction to the detection efficiency must be made before using the MC calculated efficiency to estimate the radioactivity of the source.

In this study, a novel "multi-primary coincident counting" algorithm was developed using the Geant4 Monte Carlo toolkit. An HPGe detector for ^{60}Co (two cascade gamma rays per disintegration) gamma-ray spectroscopy was accurately modeled to validate this algorithm. This ^{60}Co source option was selected over more complex coincident arrangements for its simplicity and capacity to fully demonstrate the method with a spectrum that is well understood. The simulated spectrum using the novel algorithm was compared with the measured spectrum and with the simulated spectrum using the traditional MC algorithm.

This study establishes a methodology for solving the true coincident counting issues in Monte Carlo simulations. However, because the resolving time of a detector and the time interval between two or more independent decay events from the same radioactive source cannot be modeled in the current Monte Carlo simulation, the chance coincidence counting issues cannot be solved using the algorithm developed in the current study.

MATERIALS AND METHODS

Experimental setup

A p-type closed-ended coaxial HPGe detector was used in this study as the spectrometer in the measurement (GC3518; Canberra Industries, Inc., Meriden, CT, USA). The detector configuration is shown in Fig. 1 (Canberra Industries I, 2009) (recompiled with additional notes). The diameter of the detector end-cap is 76.2 mm. The Ge crystal is housed in a vacuum environment with a 1.5-mm-thick Al protective cover. The diameter of the Ge crystal (sensitive part) is 60 mm, and the height is 51.5 mm. The diameter of the inner core is 9 mm, and the height is 34 mm. The outer n-type electrical contact of the Ge crystal is a 0.5 mm diffused Li layer, and the inner p-type electrical contact is a 0.3 μm implanted B layer. The contacts are actually dead layers for detection in which electron/hole pairs produced by energy deposition cannot be collected and do not contribute to the output pulses.

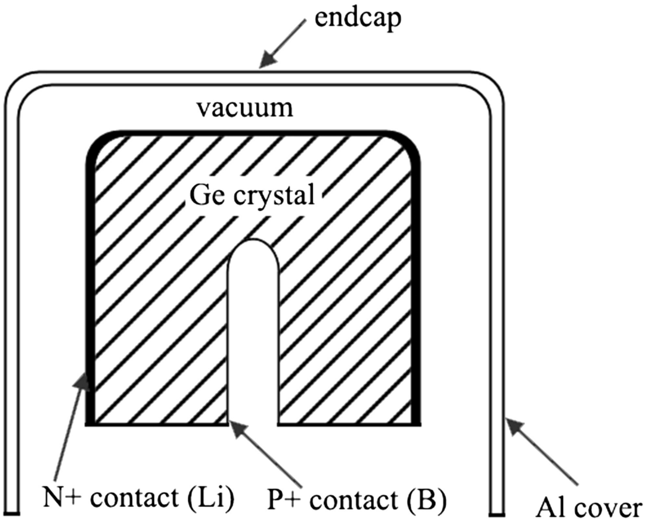

Fig. 1. Configuration of a p-type closed-ended coaxial HPGe detector.

The energy calibration factor of the GC3518 HPGe detector used in this study was obtained experimentally. The sources used for calibration included ^{57}Co, ^{60}Co, ^{88}Y, ^{109}Cd, ^{113}Sn, ^{137}Cs, and ^{139}Ba. The standard error of each gamma-ray energy point is below 1 keV. The energy calibration factor derived from the experimental data is 0.4245 ± 0.0001 keV per channel. The measured pulse height spectrum was converted to the energy deposition spectrum using this energy calibration factor.

The gamma-ray spectrum analysis experiment was performed in the Nuclear Science Center at Texas A&M University. The setup of the experiment included the HPGe detector, the lead-brick shielding walls, and the liquid nitrogen Dewar. The cutaway view of the experimental setup with simplified geometry is shown in Fig. 2.

The activity of the ^{60}Co ($T_{1/2}$ = 5.27 y) source was 5.5 kBq at the time of measurement. A long source holder (SH No.3) was used to support the source. The source was placed 9.2 cm above the end-cap of the detector (source to Ge crystal front surface distance is 9.9 cm) along the central axis of the cylindrical detector. The source dimension is much smaller than the source-to-detector surface distance, so that the point source approximation can be used reasonably. The spectrum analysis software was Genie 2000 (Canberra Industries, Inc.). The live counting time was planned to be 66 h. Due to the existence of dead time of the detector, the real counting time was 66.4 h (0.59% dead time). The total number of decays of this ^{60}Co source is 1.31×10^9 through the measurement. In addition, the background radiation was measured for 66 h using the same experimental settings without the ^{60}Co source. The electronics of the detection system were set up to detect events with energy deposition above 60 keV.

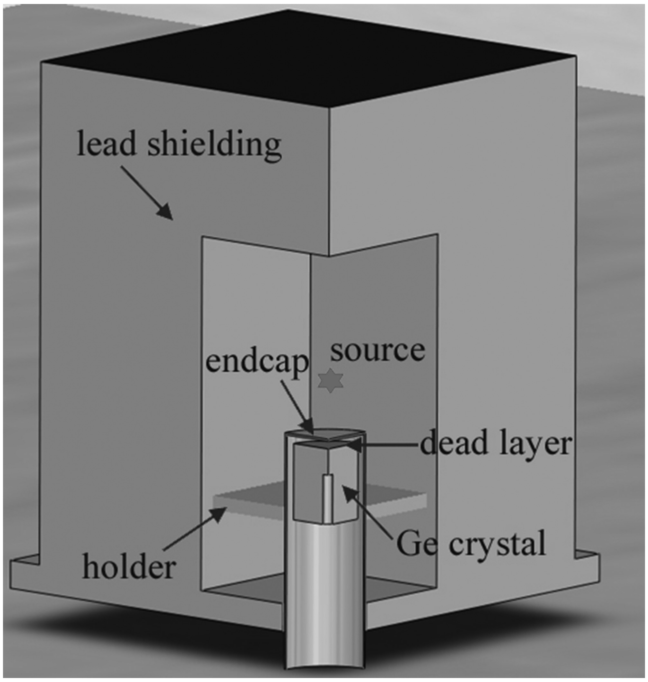

Fig. 2. The cutaway view of the experimental setup of the GC3518 HPGe detector for gamma-ray spectroscopy. The round corners of the detector end-cap and crystal shown in Fig. 1 were omitted in geometry modeling. The source holder was not depicted.

Monte Carlo simulation

A general purpose Monte Carlo toolkit, Geant4 (Agostinelli et al. 2003; Allison et al. 2006), was used as the simulation tool in this study. This tool is not a ready-to-use application like other general purpose MC codes such as MCNP(X), where the user only needs to write an input deck and implement the executable file to start a simulation (Pelowitz 2005). With Geant4, the user must create a specific project, write the source codes following both Geant4 and C++ rules, and then compile the source codes to produce an executable file to implement the simulation. Using this open-source feature, the authors developed their own algorithms to define the particle source and process counts in the HPGe detector. In addition, some precompiled external C++ libraries can be incorporated into the user's code to facilitate the storage and analysis of the simulation data. In this study, the histogram classes from a C++–based scientific data analysis tool, ROOT, were invoked in these algorithms to store and process the simulation data (Brun and Rademakers 1997).

Gamma source definition

Due to the long source-to-detector surface distance, the ^{60}Co source in the simulation was modeled as a point source, and the direction of gamma-ray emission was assumed to be isotropic. The key point in defining the gamma-ray source in this study was the specification of the number of primary gamma rays per simulation event. (In a Monte Carlo simulation, one "event" or "history" is the basic simulation unit in which all the primary particles and their secondary particles are tracked.)

In the traditional MC method, only one primary particle is emitted from the particle source per simulation event. For general problems, such as radiation shielding calculation or medical patient dose calculation, this source definition method does not cause systematic errors because the quantity of interest (i.e., accumulated dose) is proportional to the total number of simulated particle histories.

In gamma-ray spectroscopy, it is unavoidable to produce "coincident" counts in the detector due to the simultaneous detection of two or more gamma rays. However, in the traditional Monte Carlo method, only a single primary particle history can be modeled per simulation event. This intrinsic drawback makes it incapable of generating "coincident" (at least two indistinguishable detection) counts in the simulated spectrum.

In this study, a "multi-primary particle per event" source definition method was developed to model the source emitting cascade gamma rays per decay; i.e., a ^{60}Co source. In this new source definition method, when modeling a ^{60}Co source, two cascade gamma rays (1.173 MeV and 1.332 MeV) were specified deterministically in each simulation event, not sampled randomly with equal probability as in the traditional MC method. The primary source is specified in a user-defined Geant4 class derived from "G4VUserPrimaryGeneratorAction."

To show the Gaussian spread in full-energy peaks of the simulated spectrum, the source gamma-ray energy distribution was also assumed to follow a Gaussian distribution with one sigma equal to 0.766 keV for both 1.173 MeV and 1.332 MeV gamma rays (derived from the FWHM 1.8 keV at 1.332 MeV peak for the GC3518 detector).

Counting algorithms

For the spectrometer, the energy deposition events in the sensitive volume trigger the output pulse signal. Essentially, the energy depositions from gamma-ray interactions are not from gamma-ray trajectories directly but from the secondary electron trajectories. Ideally, the detector collects all the energy depositions from an incident primary gamma ray and all of its offspring particles (electrons, positrons, or photons) in the sensitive volume and converts the sum energy to an output pulse. In cases with two or more gamma rays interacting with the detector in coincidence, the detector collects the sum energy deposition from coincident gamma rays and all of their offspring particles rather than treating them separately. Hence, the "sum peak" and "sum continuum" are observed in a real measured spectrum. The measured pulse height spectrum can be converted to the energy deposition spectrum using the energy calibration factor mentioned above.

In a Monte Carlo calculation, only the energy deposition can be collected rather than the pulse height. Hence, the counting algorithm plays an important role in determining the shape of the simulated energy deposition spectrum. The effectiveness of a Monte Carlo algorithm can be validated experimentally. For an effective algorithm, the shape of the simulated spectrum should agree with the measured spectrum, at least qualitatively.

The traditional and coincident Monte Carlo counting algorithms for a ^{60}Co source developed using Geant4 are compared in Table 1, and the results comparison will be discussed in a later section.

The processes to produce counts using the traditional MC algorithm are described below:

1. Assign the track ID number of the primary gamma ray to all of its offspring particles as their unique identification, original track ID number, which is always “1” because only one primary is generated in each event;
2. The tracking steps with the same original track ID number make contributions to the same output signal, total energy deposition per simulation event;
3. If there is no energy deposition in this event, there is no output signal. If the total energy deposition per event is a positive value, one count is filled in the corresponding energy channel in the pre-defined ROOT histogram; and
4. After all events are processed, the energy deposition spectrum is dumped into a binary ROOT file.

The processes to produce counts using the coincident MC algorithm are described below:

1. Assign the track ID number of each primary gamma ray to all of its offspring particles as their unique identification, original track ID number, respectively. For a ^{60}Co source, these two original track ID numbers are “1” and “2” corresponding to the two cascade gamma rays;
2. The tracking steps with different original track ID numbers make contributions to the same output signal—total energy deposition per simulation event. If the total energy deposition in this event is accidently from tracks with two different original track ID numbers, it means “coincident” counting from the two original cascade gamma rays happens;
3. If there is no energy deposition in this event, there is no output signal. If the total energy deposition per event is a positive value, one count is filled in the corresponding energy channel in the pre-defined ROOT histogram; and
4. After all events are processed, the energy deposition spectrum is dumped into a binary ROOT file.

The track ID assignment is processed by invoking two user-defined Geant4 classes derived from “G4VUserTrackInformation” and “G4UserTrackingAction.” The energy deposition accumulation in each simulation event is processed by invoking user-defined Geant4 classes derived from “G4VHit” and “G4VSensitiveDetector.”

In summary, the differences between the traditional and coincident MC algorithms are the first two steps: gamma-ray source definition and energy deposition collection.

RESULTS AND DISCUSSION

The simulated spectra produced from the traditional and coincident MC algorithms were compared in this study. The simulated spectrum produced using the coincident MC algorithm was also compared with the measured spectrum.

Comparison between simulated spectra from two counting algorithms

The simulated spectra from the traditional MC algorithm and the coincident MC algorithm are compared in Fig. 3. The counts in the spectra are the absolute counts per channel. The number of simulated gamma rays was 1.31×10^9 for either peak energy of the two cascade gamma rays emitted from the ^{60}Co source in both algorithms. The most obvious difference between these two spectra is the “summation effect.” In the spectrum from the traditional MC algorithm, there are no counts in the channels after the 1.332 MeV full-energy peak. In the spectrum from the coincident MC algorithm, the coincident counts are very obvious starting from the middle region of the multiple Compton events between the two full-energy peaks and ending at the 2.5 MeV sum peak.

Comparison between the simulated spectrum from coincident MC algorithm and the measured spectrum

The simulated spectrum from the “multi-primary coincident counting” algorithm and the measured spectrum

Table 1. Comparison of the traditional and coincident MC algorithms.

	Traditional MC	Coincident MC
Number of gamma rays per simulation event	One 1.173 MeV gamma ray **or** one 1.332 MeV gamma ray	One 1.173 MeV gamma ray **and** one 1.332 MeV gamma ray
Data collection	Contribution from **one** primary gamma ray and its secondary radiations	Total contribution from **two** primary gamma rays and their secondary radiations
Coincident counts	Not considered	Considered

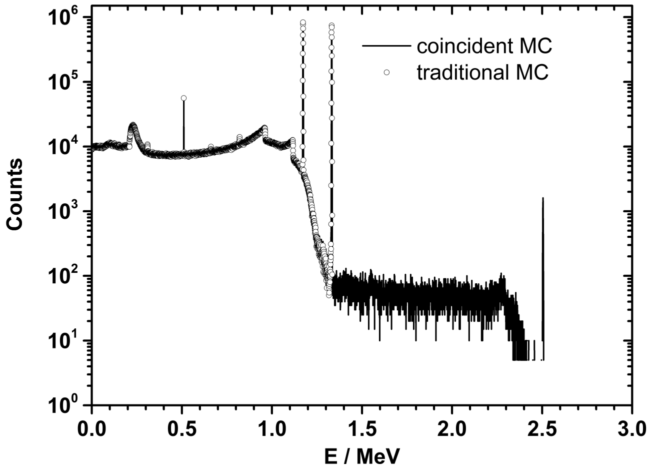

Fig. 3. Comparison of the simulated spectra using the traditional MC and coincident MC algorithms. The spectrum from traditional MC is plotted with circle holes; the spectrum from coincident MC is plotted with a black solid line.

with net counts in each channel (net counts = total counts − background counts) are compared in Fig. 4.

Overall, the two spectra show excellent agreement qualitatively, and both indicate a coincident sum continuum and a sum peak. However, due to the long source-to-surface distance, the geometry factor is low, resulting in the low probability of coincident counts. Hence, there are large fluctuations in the sum continuum on both spectra. In the measured spectrum, there are counts in the energy channels above the sum peak at 2.5 MeV, which are probably caused by the chance coincident events. The simulation shows a much higher annihilation peak at 511 keV, which may be due to the high interaction cross sections used in the Geant4 MC code. Below the annihilation peak energy, there are more counts in the measured spectrum than in the simulated spectrum. The reason is unknown. There are more counts under full-energy peaks in the simulated spectrum than in the measured spectrum. Hence, the simulation using the coincident MC algorithm still overestimates the detection efficiency for either specific gamma-ray energy. In addition, the simulated spectrum using the "multi-primary coincident counting" algorithm is qualitatively comparable with the experimental spectrum in other studies (Knoll 2010).

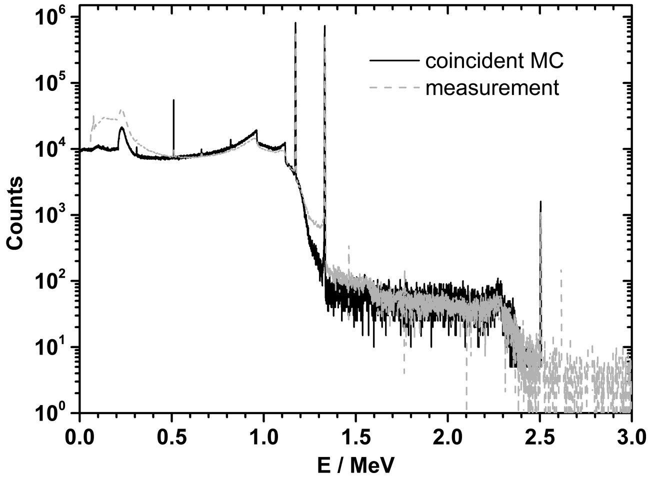

Fig. 4. Comparison of the simulated spectra using the coincident MC algorithm and the measured spectrum. The spectrum from coincident MC is plotted with a black solid line; the spectrum from measurement is plotted with a gray dash line.

Detection efficiency comparison

If the full-energy peak is superimposed on a counting continuum, the unwanted counts in the continuum should be subtracted when calculating the detection efficiency for this specific gamma-ray energy. Based on this counting method, the calculated absolute full-energy peak efficiency for measurement, traditional MC algorithm, and coincident MC algorithm are compared in Table 2. The results show that the Monte Carlo methods overestimate the detection efficiency, and detection efficiency from the traditional MC method is higher than the result from the coincident MC algorithm, mainly due to the neglect of "coincident counts." Similar results [that the MC algorithm predicted higher detection efficiency than measurement (Vasconcelos et al. 2011)] were also obtained in other studies.

CONCLUSION

This work describes a novel "multi-primary coincident counting" Monte Carlo algorithm developed for simulating the detection of cascade gamma rays. The method was demonstrated using a simulated pulse height spectrum for ^{60}Co. The "coincident counting" method showed excellent qualitative agreement with the measured ^{60}Co spectrum using a closed-ended coaxial HPGe detector.

The selection of ^{60}Co spectroscopy using an HPGe detector is due to its simplicity and well-known spectrum characteristics. Similarly, the developed methodology can be extended to more complex applications with high "coincident" hitting rate from multiple types of radiations, such as in the process of nuclear fission and used nuclear fuel with multiple neutrons and gamma rays emitted in coincidence. For other applications, the basic principle in defining the primary source is same as the one developed in this study. The only needed modification is specifying the number and type of initial radiations in the Geant4 C++ "source definition" class accordingly, but the developed "coincident detection" class can be used directly without modification.

Table 2. The calculated absolute full-energy peak efficiency for measurement, traditional MC algorithm, and coincident MC algorithm.

	Absolute full-energy peak efficiency		
E_γ (MeV)	Measurement	Traditional MC	Coincident MC
1.173	2.27×10^{-3}	2.91×10^{-3}	2.87×10^{-3}
1.332	2.06×10^{-3}	2.62×10^{-3}	2.58×10^{-3}

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